

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -76.6 °C

Global applicability domain: Inside

Local applicability domain index: 7.64e-01

Confidence level: 5.94e-01

Nearest Neighbors from the Training Set

Image not found

Acrolein

Measured: -87.7

Predicted: -76.6

Image not found

Methacrylaldehyde

Measured: -81.0

Predicted: -62.4

Image not found

(E)-Crotonaldehyde

Measured: -76.3

Predicted: -60.8

Image not found

Crotonaldehyde

Measured: -76.3

Predicted: -60.8

Image not found

1-Chloro-3,3-dimethyl-butan-2-one

Measured: -13.0

Predicted: -41.1

Image not found

Hexanoyl chloride

Measured: -87.0

Predicted: -73.0